Supplementary information

Defect and carrier characteristics of chalcogenide perovskite $BaZrS_3$ under thermodynamically stability: A first-principles study for photovoltaic application

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Optical characteristics of $BaZrS_3$:

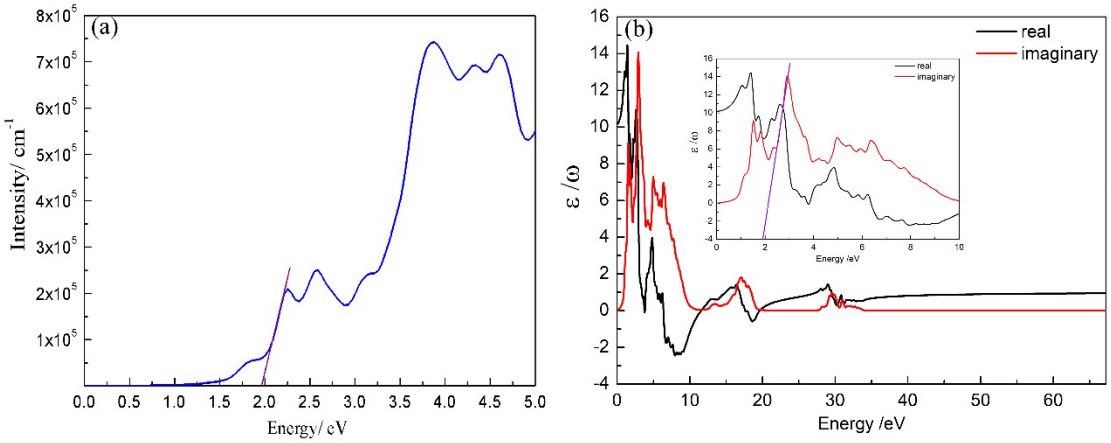

Figure S1. Calculated (a) optical absorption and (b) dielectric constant characteristics of $BaZrS_3$.

Influence of element doping on the band and thermodynamically stability of $BaZrS_3$:

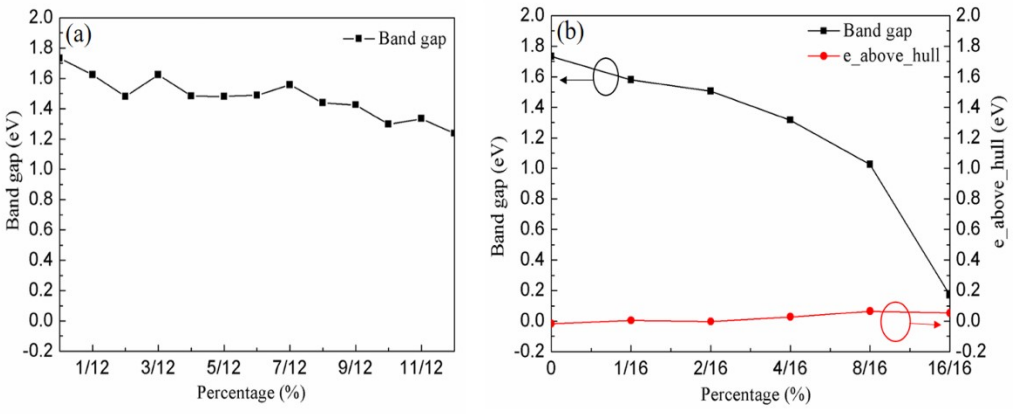

Figure S2. (a) The band gap of $BaZrS_3$ with the varied Se doping; (b) The band gap and e_above_hull of $BaZrS_3$ with the varied Ti doping.

Formation energy of intrinsic defects in $BaZrS_3$ as a function of the Fermi energy:

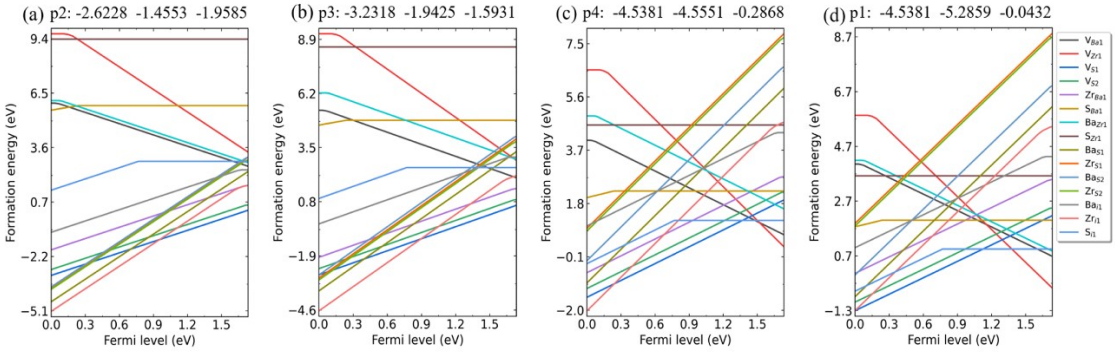

Figure S3. The formation energy of intrinsic defects as a function of the Fermi energy in the sequence of p2-p3-p4-p1, as displayed in (a)-(b)-(c)-(d). The defect charge state determines the slope of the line, and the turning points represent the transition energy levels between different charge states for a given defect.

Photoelectric conversion characteristics of the modeled $BaZrS_3$ solar cell:

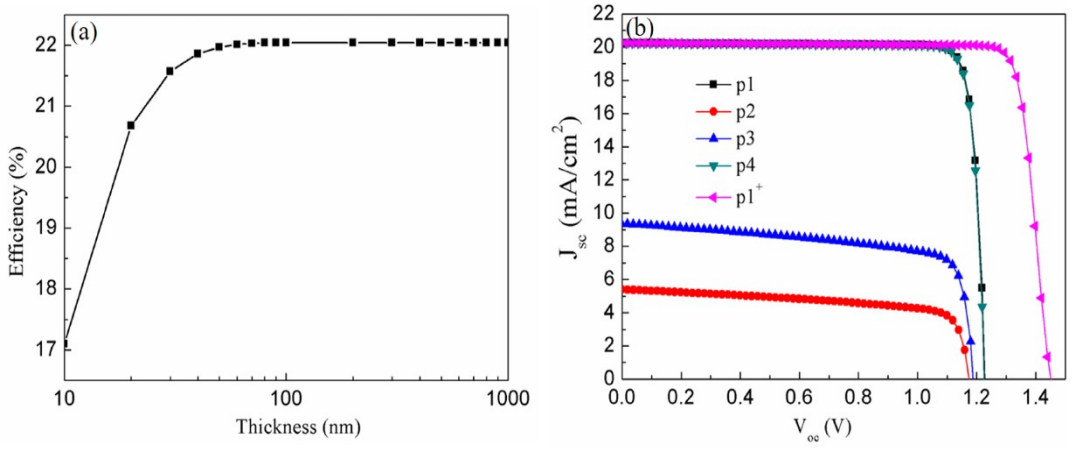

Figure S4. The calculated J-V characteristics of $BaZrS_3$ in the $BaZrS_3$-PTAA junction. (a) The effect of thin-film thickness of the $BaZrS_3$ on its conversion efficiency; (b) the photovoltaic properties of $BaZrS_3$ at p2, p3, p4, p1 and $p1^+$.

Table S1. The main photoelectric features of $BaZrS_3$.

	p2	**p3**	**p4**	**p1**	**$p1^+$**
Efficiency	4.34 %	7.96%	21.96%	22.04 %	25.46%
Short-circuit current (J_{sc}, mA/cm^2)	5.41	9.37	20.24	20.25	20.25
Open circuit voltage (V_{oc}, V)	1.17	1.19	1.23	1.228	1.45
Fill factor (FF, %)	68.40	71.43	88.46	88.61	86.73